



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:19 pm BST

PDB ID : 2CEQ  
Title : Beta-glycosidase from *Sulfolobus solfataricus* in complex with glucoimidazole  
Authors : Gloster, T.M.; Moracci, M.; Vasella, A.; Davies, G.J.  
Deposited on : 2006-02-10  
Resolution : 2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

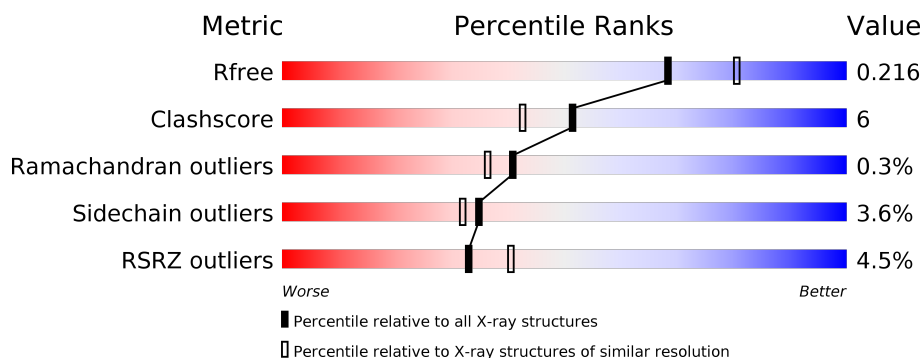
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	489	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9121 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	22	0
			4106	2649	696	746	15			
1	B	489	Total	C	N	O	S	0	20	0
			4091	2636	697	745	13			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



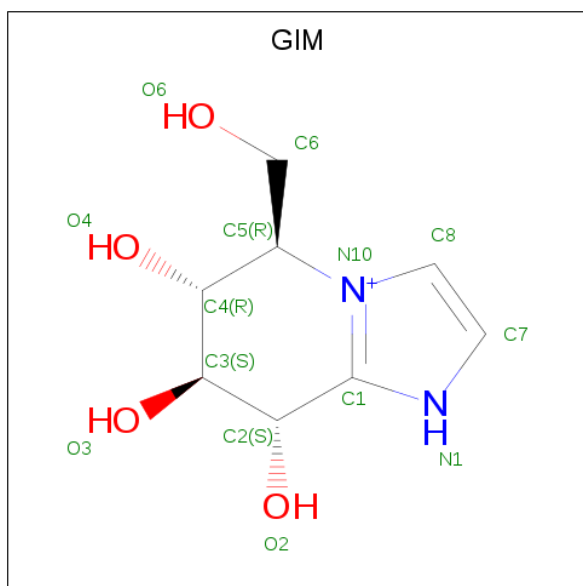
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLUCOIMIDAZOLE (three-letter code: GIM) (formula:  $C_8H_{13}N_2O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	2	4		
3	B	1	Total	C	N	O	0	0
			14	8	2	4		

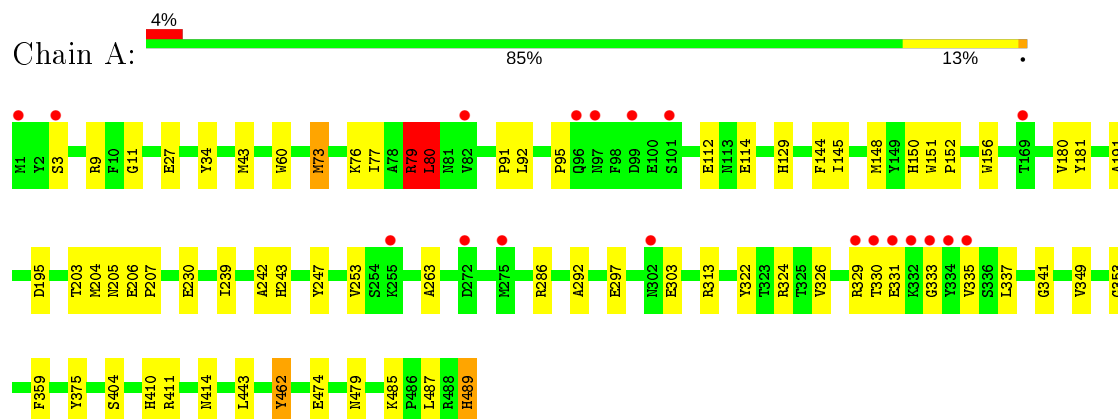
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	442	Total	O	0	0
			442	442		
4	B	434	Total	O	0	0
			434	434		

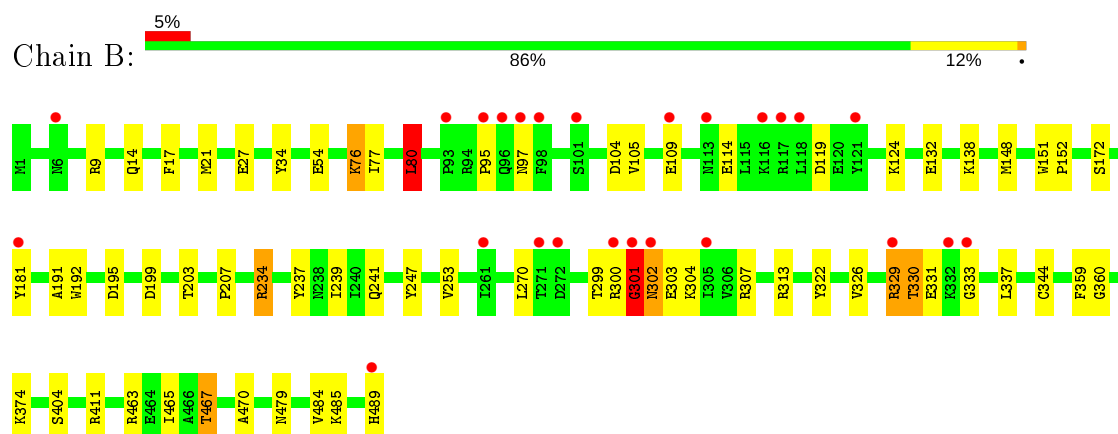
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: BETA-GALACTOSIDASE



#### • Molecule 1: BETA-GALACTOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.93 Å   167.93 Å   93.42 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	145.86 – 2.14 39.30 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.4 (145.86-2.14) 99.4 (39.30-2.14)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.14 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.176 , 0.215 0.178 , 0.216	Depositor DCC
$R_{free}$ test set	4163 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GIM, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	0/4302	0.67	2/5839 (0.0%)
1	B	0.71	2/4280 (0.0%)	0.67	3/5810 (0.1%)
All	All	0.68	2/8582 (0.0%)	0.67	5/11649 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76[A]	LYS	C-O	15.28	1.52	1.23
1	B	76[B]	LYS	C-O	15.28	1.52	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	301	GLY	N-CA-C	-8.04	92.99	113.10
1	A	79	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	B	80	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	80	LEU	CA-CB-CG	6.62	130.53	115.30
1	B	302	ASN	N-CA-C	-5.47	96.23	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	300	ARG	Peptide
1	B	301	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4106	0	3958	45	0
1	B	4091	0	3937	46	0
2	A	8	0	6	0	0
2	B	12	0	9	0	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
4	A	442	0	0	8	0
4	B	434	0	0	4	0
All	All	9121	0	7936	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485[B]:LYS:NZ	4:A:2438:HOH:O	1.85	1.05
1:B:76[A]:LYS:NZ	4:B:2108:HOH:O	2.01	0.92
1:B:9[B]:ARG:NH2	4:B:2014:HOH:O	1.58	0.91
1:B:14:GLN:HG2	1:B:80:LEU:HD12	1.53	0.90
1:B:234[A]:ARG:NH1	4:B:2240:HOH:O	2.09	0.86
1:B:463:ARG:O	1:B:467:THR:HB	1.77	0.83
1:A:95:PRO:HB3	1:A:181[B]:TYR:CE2	2.16	0.80
1:A:27[B]:GLU:OE2	1:A:34:TYR:OH	1.98	0.80
1:B:104:ASP:HA	1:B:241:GLN:HE22	1.50	0.76
1:A:485[B]:LYS:CE	4:A:2438:HOH:O	2.31	0.69
1:A:43:MET:HE1	4:A:2069:HOH:O	1.93	0.69
1:B:95:PRO:HG2	1:B:181:TYR:CE1	2.29	0.67
1:B:241:GLN:HE21	1:B:307:ARG:HH22	1.43	0.66
1:A:485[B]:LYS:HE2	4:A:2438:HOH:O	1.95	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73[A]:MET:CE	1:A:443:LEU:HD13	2.25	0.65
1:B:301:GLY:C	1:B:303:GLU:H	2.01	0.62
1:A:349:VAL:CG1	1:A:353:GLY:HA2	2.30	0.62
1:B:299:THR:HG23	1:B:302:ASN:H	1.63	0.62
1:A:80:LEU:HD22	1:A:144:PHE:HE1	1.65	0.62
1:B:138[A]:LYS:NZ	1:B:199:ASP:OD2	2.27	0.60
1:B:191:ALA:O	1:B:195:ASP:HB2	2.02	0.59
1:B:301:GLY:CA	1:B:302:ASN:HB2	2.32	0.59
1:B:14:GLN:HG2	1:B:80:LEU:CD1	2.31	0.58
1:A:73[A]:MET:HE2	1:A:443:LEU:HD13	1.86	0.57
1:B:270:LEU:HD22	1:B:337:LEU:HD11	1.89	0.55
1:A:204[B]:MET:HE3	1:A:207:PRO:HG3	1.88	0.54
1:B:207:PRO:CB	1:B:239[B]:ILE:HG21	2.40	0.52
1:A:95:PRO:CB	1:A:181[B]:TYR:CE2	2.92	0.52
1:A:330:THR:CG2	1:A:331:GLU:N	2.73	0.52
1:B:484:VAL:O	1:B:489:HIS:HE1	1.92	0.52
1:A:230:GLU:HG3	4:A:2254:HOH:O	2.10	0.51
1:A:326:VAL:HG12	1:A:337:LEU:HD12	1.94	0.50
1:A:206:GLU:CD	1:A:263:ALA:HB2	2.32	0.50
1:A:349:VAL:HG13	1:A:353:GLY:HA2	1.93	0.50
1:A:73[A]:MET:HE1	1:A:443:LEU:HD13	1.95	0.49
1:B:105:VAL:H	1:B:241:GLN:NE2	2.11	0.49
1:B:247:TYR:CD1	1:B:313:ARG:HG3	2.47	0.49
1:B:344:CYS:HB2	1:B:360:GLY:O	2.13	0.48
1:B:241:GLN:NE2	1:B:307:ARG:HH12	2.11	0.48
1:B:76[B]:LYS:HD3	1:B:76[B]:LYS:HA	1.91	0.47
1:A:79:ARG:NH2	1:A:205:ASN:OD1	2.44	0.47
1:A:60:TRP:O	1:A:129:HIS:HE1	1.97	0.47
1:A:148:MET:HB2	1:A:203:THR:O	2.15	0.47
1:A:73[A]:MET:HE3	1:A:462:TYR:HB3	1.96	0.47
1:A:91:PRO:HA	1:A:156:TRP:CD2	2.49	0.47
1:B:21:MET:HB3	1:B:54:GLU:HA	1.97	0.47
1:B:241:GLN:HE21	1:B:307:ARG:HH12	1.63	0.47
1:B:27[B]:GLU:OE2	1:B:34:TYR:OH	2.24	0.47
1:A:150:HIS:O	1:A:152:PRO:HD3	2.16	0.46
1:B:237:TYR:O	1:B:241:GLN:HG3	2.16	0.46
1:A:11:GLY:HA3	1:A:77:ILE:O	2.16	0.46
1:A:204[B]:MET:HE2	1:A:243:HIS:HB2	1.98	0.46
1:A:60:TRP:O	1:A:129:HIS:CE1	2.68	0.46
1:B:192:TRP:HA	1:B:253[A]:VAL:HG11	1.97	0.46
1:B:207:PRO:HB3	1:B:239[B]:ILE:HG21	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:TYR:CD1	1:A:313:ARG:HG3	2.50	0.46
1:A:286:ARG:HD3	4:A:2294:HOH:O	2.16	0.46
1:B:301:GLY:HA2	1:B:302:ASN:HB2	1.96	0.46
1:B:330:THR:HG23	1:B:331:GLU:N	2.31	0.45
1:A:286:ARG:HD2	1:A:375:TYR:CZ	2.52	0.45
1:A:76[B]:LYS:NZ	4:A:2107:HOH:O	2.42	0.45
1:A:322:TYR:CE2	3:A:1492:GIM:C8	3.00	0.45
1:B:17:PHE:HB2	1:B:152:PRO:HG2	1.98	0.45
1:A:292:ALA:HA	1:A:297:GLU:O	2.17	0.45
1:B:76[B]:LYS:O	1:B:77:ILE:N	2.50	0.45
1:B:76[B]:LYS:HB2	4:B:2020:HOH:O	2.16	0.44
1:A:79:ARG:HB2	1:A:145:ILE:HB	1.99	0.44
1:B:404:SER:HA	1:B:479:ASN:HD22	1.82	0.44
1:B:326:VAL:HG12	1:B:337:LEU:HD12	2.00	0.43
1:A:73[A]:MET:CE	1:A:462:TYR:HD2	2.31	0.43
1:A:404:SER:HA	1:A:479:ASN:HD22	1.83	0.43
1:B:148:MET:HB2	1:B:203:THR:O	2.19	0.43
1:B:207:PRO:HB2	1:B:239[B]:ILE:HG21	2.00	0.43
1:A:180:VAL:HG13	1:A:242:ALA:HA	2.00	0.42
1:A:191:ALA:O	1:A:195:ASP:HB2	2.20	0.42
1:B:241:GLN:HE21	1:B:307:ARG:NH2	2.13	0.41
1:B:322:TYR:CE2	3:B:1493:GIM:C8	3.03	0.41
1:A:324:ARG:O	1:A:341:GLY:HA3	2.20	0.41
1:A:489:HIS:N	1:A:489:HIS:CD2	2.88	0.41
1:A:95:PRO:HB3	1:A:181[B]:TYR:CZ	2.52	0.41
1:A:80:LEU:HD22	1:A:144:PHE:CE1	2.48	0.41
1:B:465:ILE:HA	1:B:470:ALA:O	2.21	0.41
1:A:487:LEU:O	1:A:489:HIS:CD2	2.73	0.41
1:B:119:ASP:O	1:B:124:LYS:NZ	2.53	0.41
1:B:97:ASN:ND2	1:B:97:ASN:H	2.17	0.41
1:A:9[B]:ARG:HD2	4:A:2014:HOH:O	2.21	0.40
1:B:329:ARG:HD3	1:B:333:GLY:O	2.21	0.40
1:B:76[B]:LYS:CA	1:B:77:ILE:N	2.83	0.40
1:A:3:SER:O	1:A:410:HIS:NE2	2.54	0.40
1:B:330:THR:CG2	1:B:331:GLU:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/489 (104%)	494 (97%)	12 (2%)	2 (0%)	34	29
1	B	507/489 (104%)	492 (97%)	14 (3%)	1 (0%)	47	45
All	All	1015/978 (104%)	986 (97%)	26 (3%)	3 (0%)	41	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	B	151	TRP
1	A	333	GLY

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/421 (104%)	420 (96%)	18 (4%)	30	27
1	B	436/421 (104%)	420 (96%)	16 (4%)	34	31
All	All	874/842 (104%)	840 (96%)	34 (4%)	35	29

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73[A]	MET
1	A	73[B]	MET
1	A	79	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	80	LEU
1	A	92	LEU
1	A	112	GLU
1	A	114	GLU
1	A	239	ILE
1	A	253	VAL
1	A	303	GLU
1	A	329	ARG
1	A	335	VAL
1	A	359	PHE
1	A	411	ARG
1	A	414	ASN
1	A	462	TYR
1	A	474	GLU
1	A	489	HIS
1	B	80	LEU
1	B	109	GLU
1	B	114	GLU
1	B	172[A]	SER
1	B	172[B]	SER
1	B	234[A]	ARG
1	B	234[B]	ARG
1	B	304	LYS
1	B	329	ARG
1	B	330	THR
1	B	359	PHE
1	B	374	LYS
1	B	411	ARG
1	B	467	THR
1	B	485[A]	LYS
1	B	485[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	128	ASN
1	A	129	HIS
1	A	264	ASN
1	A	388	ASN
1	A	430	ASN
1	A	479	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	489	HIS
1	B	97	ASN
1	B	103	GLN
1	B	241	GLN
1	B	430	ASN
1	B	479	ASN
1	B	489	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACT	A	1491	-	1,3,3	1.57	0	0,3,3	0.00	-
2	ACT	B	1491	-	1,3,3	1.65	0	0,3,3	0.00	-
2	ACT	B	1492	-	1,3,3	1.28	0	0,3,3	0.00	-
2	ACT	A	1490	-	1,3,3	1.72	0	0,3,3	0.00	-
2	ACT	B	1490	-	1,3,3	0.72	0	0,3,3	0.00	-
3	GIM	A	1492	-	13,15,15	0.65	0	11,22,22	1.03	1 (9%)
3	GIM	B	1493	-	13,15,15	0.84	1 (7%)	11,22,22	0.97	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GIM	B	1493	-	-	0/2/22/22	0/1/2/2
3	GIM	A	1492	-	-	0/2/22/22	0/1/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1493	GIM	C8-N10	-2.01	1.34	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1492	GIM	C3-C4-C5	-2.65	106.90	111.37
3	B	1493	GIM	C3-C4-C5	-2.16	107.72	111.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1492	GIM	1	0
3	B	1493	GIM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	489/489 (100%)	0.01	19 (3%)	39 47	23, 33, 52, 69	0
1	B	489/489 (100%)	0.03	25 (5%)	28 34	20, 33, 55, 71	1 (0%)
All	All	978/978 (100%)	0.02	44 (4%)	33 40	20, 33, 54, 71	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96[A]	GLN	6.1
1	B	98	PHE	5.5
1	B	301	GLY	5.3
1	B	97	ASN	5.2
1	A	332	LYS	3.8
1	A	333	GLY	3.7
1	A	329	ARG	3.7
1	B	113	ASN	3.4
1	B	6	ASN	3.4
1	B	117	ARG	3.4
1	B	93	PRO	3.3
1	A	97	ASN	3.2
1	B	121	TYR	3.1
1	A	330	THR	3.1
1	A	96	GLN	3.1
1	A	335	VAL	3.1
1	A	275	MET	3.0
1	B	272	ASP	3.0
1	A	272	ASP	3.0
1	B	118	LEU	3.0
1	B	95	PRO	2.9
1	B	261	ILE	2.9
1	B	305	ILE	2.9
1	A	82[A]	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	101	SER	2.8
1	B	302	ASN	2.7
1	B	489	HIS	2.7
1	B	116	LYS	2.6
1	B	300	ARG	2.5
1	B	329	ARG	2.5
1	A	255[A]	LYS	2.5
1	A	334	TYR	2.3
1	A	331	GLU	2.3
1	A	101	SER	2.2
1	A	1[A]	MET	2.2
1	B	109	GLU	2.2
1	A	302	ASN	2.1
1	B	333	GLY	2.1
1	B	271	THR	2.1
1	B	181	TYR	2.1
1	A	3	SER	2.0
1	B	332	LYS	2.0
1	A	99	ASP	2.0
1	A	169	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	A	1491	4/4	0.55	0.25	73,74,74,74	0
2	ACT	A	1490	4/4	0.73	0.30	63,63,63,63	0
2	ACT	B	1491	4/4	0.74	0.36	57,58,58,59	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACT	B	1490	4/4	0.93	0.20	59,59,59,59	0
2	ACT	B	1492	4/4	0.95	0.13	61,62,62,62	0
3	GIM	B	1493	14/14	0.97	0.18	22,26,30,31	0
3	GIM	A	1492	14/14	0.98	0.15	22,26,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.